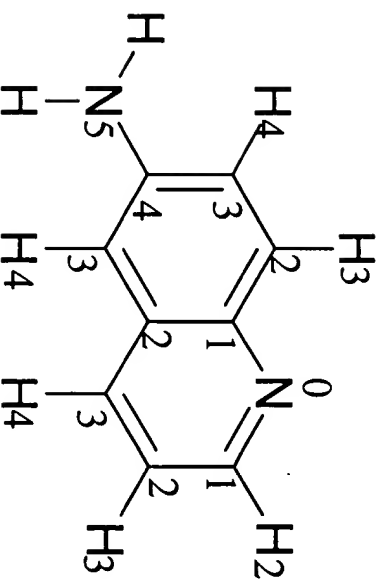


FIG. 2

ATOM TYPES

C.3	sp ³ carbon	H	hydrogen
C.2	sp ² carbon	F	fluorine
C.1	sp ¹ carbon	CL	chlorine
C.ar	aromatic carbon	BR	bromine
C.cat	cationic carbon	I	iodine
N.3	sp ³ nitrogen		
N.2	sp ² nitrogen	<u>Group Types</u>	
N.1	sp ¹ nitrogen	NO ₂	
N.ar	aromatic nitrogen	NO	
N.am	amide nitrogen	CN	
N.pl3	planar sp ³ nitrogen	CO	
N.4	protonated sp ³ nitrogen	SO ₂	
O.3	sp ³ oxygen	SO	
O.2	sp ² oxygen	OH	
O.CO2	oxygen in carboxylate and phosphate groups		
S.3	sp ³ sulfur		
S.2	sp ² sulfur		
S.O	sulfoxide sulfur		
S.O2	sulfone sulfur		
P.3	sp ³ phosphorous		



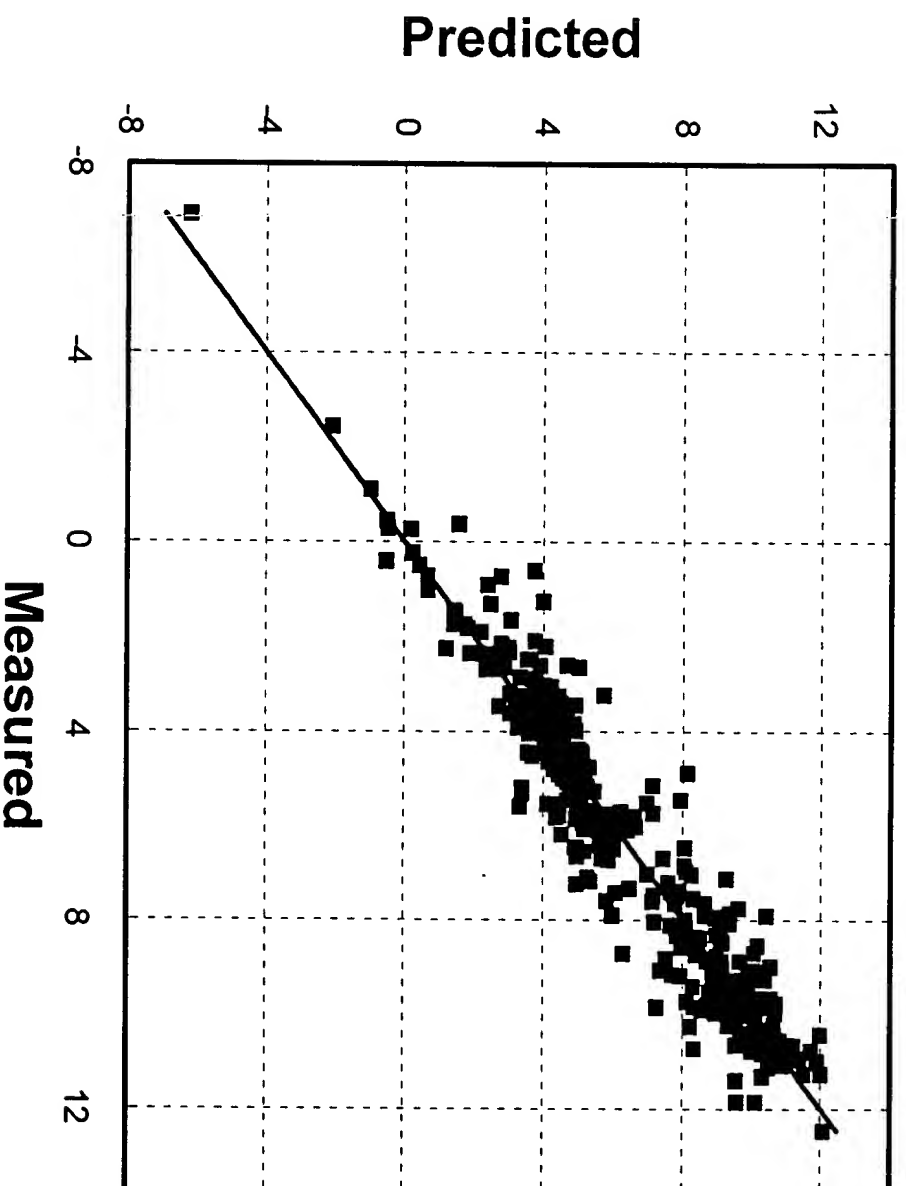
No. of atoms of certain type at each level

	N.ar	C.ar	H	N.pl3
<i>Level 0</i>	1			
<i>Level 1</i>		2		
<i>Level 2</i>		3	1	
<i>Level 3</i>		3	2	
<i>Level 4</i>		1	3	
<i>Level 5</i>				1

Construction of the hierarchical tree from one example, 6-amino quinoline

pK_a of Bases (384)

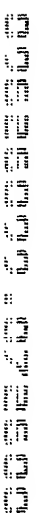
PC = 5, $r^2=0.922$ $q^2=0.832$, Std. Err = 0.89



F15.7

Run	Time	Temp	Pressure	Flow	Conc	Yield	Product
1	10	100	100	100	100	100	100
2	20	100	100	100	100	100	100
3	30	100	100	100	100	100	100
4	40	100	100	100	100	100	100
5	50	100	100	100	100	100	100
6	60	100	100	100	100	100	100
7	70	100	100	100	100	100	100
8	80	100	100	100	100	100	100
9	90	100	100	100	100	100	100
10	100	100	100	100	100	100	100
11	110	100	100	100	100	100	100
12	120	100	100	100	100	100	100
13	130	100	100	100	100	100	100
14	140	100	100	100	100	100	100
15	150	100	100	100	100	100	100
16	160	100	100	100	100	100	100
17	170	100	100	100	100	100	100
18	180	100	100	100	100	100	100
19	190	100	100	100	100	100	100
20	200	100	100	100	100	100	100
21	210	100	100	100	100	100	100
22	220	100	100	100	100	100	100
23	230	100	100	100	100	100	100
24	240	100	100	100	100	100	100
25	250	100	100	100	100	100	100
26	260	100	100	100	100	100	100
27	270	100	100	100	100	100	100
28	280	100	100	100	100	100	100
29	290	100	100	100	100	100	100
30	300	100	100	100	100	100	100
31	310	100	100	100	100	100	100
32	320	100	100	100	100	100	100
33	330	100	100	100	100	100	100
34	340	100	100	100	100	100	100
35	350	100	100	100	100	100	100
36	360	100	100	100	100	100	100
37	370	100	100	100	100	100	100
38	380	100	100	100	100	100	100
39	390	100	100	100	100	100	100
40	400	100	100	100	100	100	100
41	410	100	100	100	100	100	100
42	420	100	100	100	100	100	100
43	430	100	100	100	100	100	100
44	440	100	100	100	100	100	100
45	450	100	100	100	100	100	100
46	460	100	100	100	100	100	100
47	470	100	100	100	100	100	100
48	480	100	100	100	100	100	100
49	490	100	100	100	100	100	100
50	500	100	100	100	100	100	100
51	510	100	100	100	100	100	100
52	520	100	100	100	100		

PC = 6, $r^2 = 0.927$, $q^2 = 0.792$, Std. Err = 0.77



F15.8

examples, and were not included in the training set

Calculated pK_a

Measured pK_a

By Model

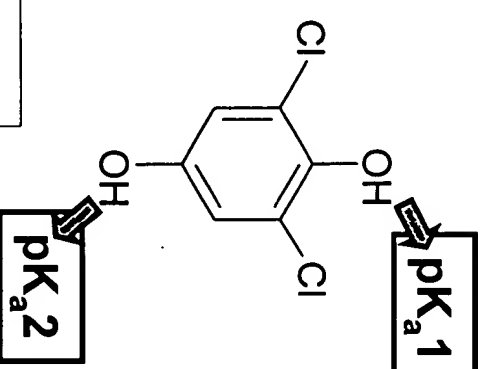
By Perrin

Predicted- r^2 Std. Err.
Model: 0.91 0.95

Oc1cc(Cl)c(Cl)c(Cl)c1

pK_{a1}

pK_{a2}

[illegible]